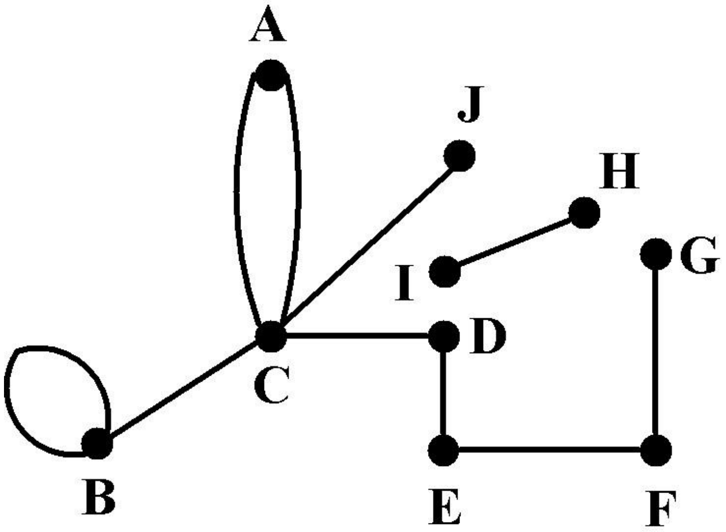
Graph concepts

Graphs are made up by vertices (nodes) and edges (links).

An edge connects two vertices, or a vertex with itself – loop.



AC, AC - multiple edges

BB – loop

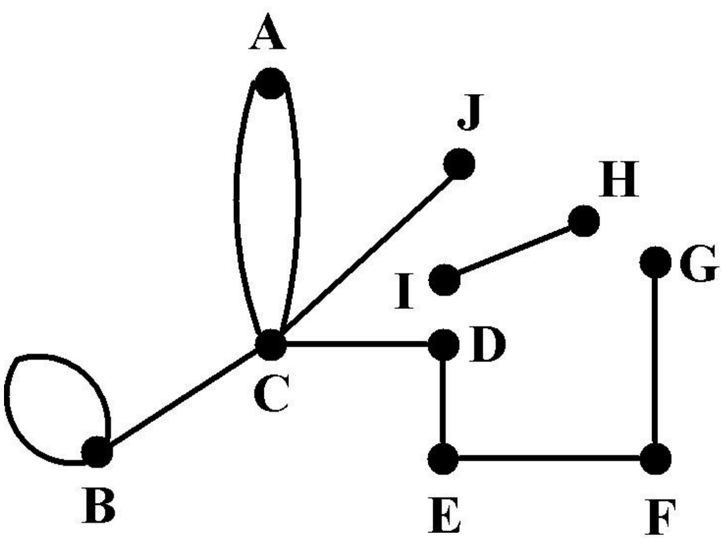
The shape of the graph does not matter, only the way the nodes are connected to each other.

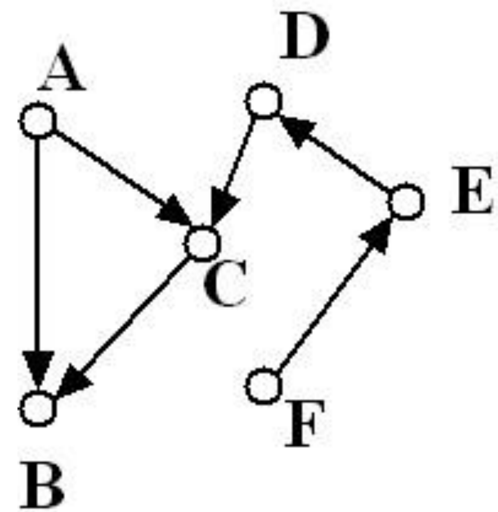
Simple graph - does not have loops (self-edges) and does not have multiple identical edges.

Further reading:
http://www.utm.edu/departments/math/graph/glossary.html

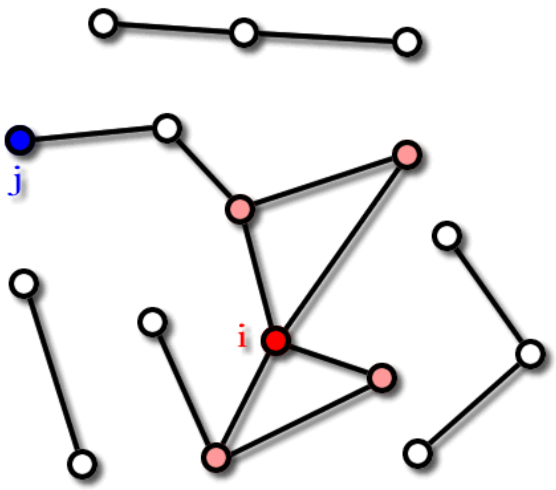
Symmetrical and directed graphs

Two distinct types of edges: symmetrical and directed (also called arcs).
Two different graph frameworks: graph, digraph = directed graph.
In the digraph framework a symmetrical edge means the superposition of two opposite directed edges.



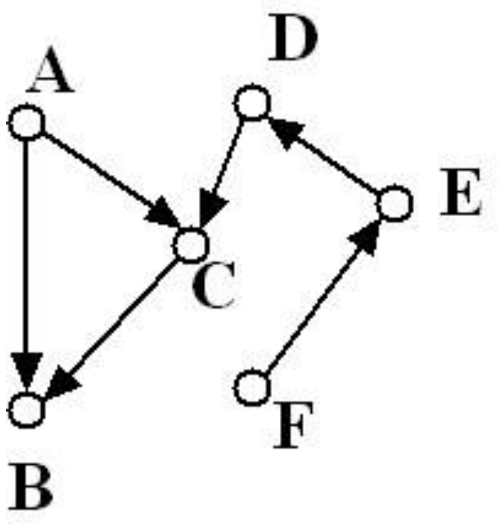


Node degrees



Node degree: the number of edges connected to the node. $k_i = 4$

In directed networks we can define an in- degree and out-degree. The (total) degree is the sum of in- and out-degree. $k_C^{in} = 2$ $k_C^{out} = 1$ $k_C = 3$

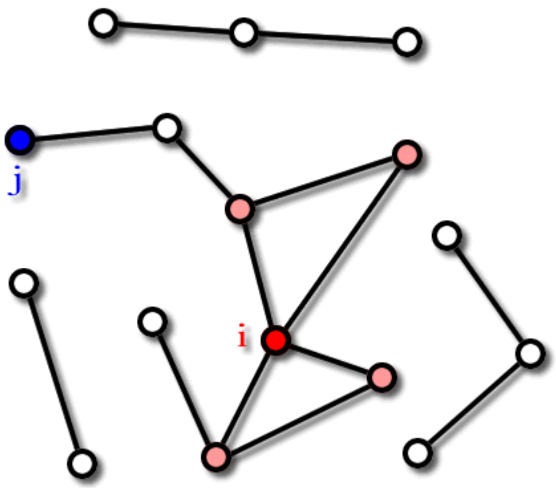


Source: a node with in-degree = 0.

Sink: a node with out-degree = 0.

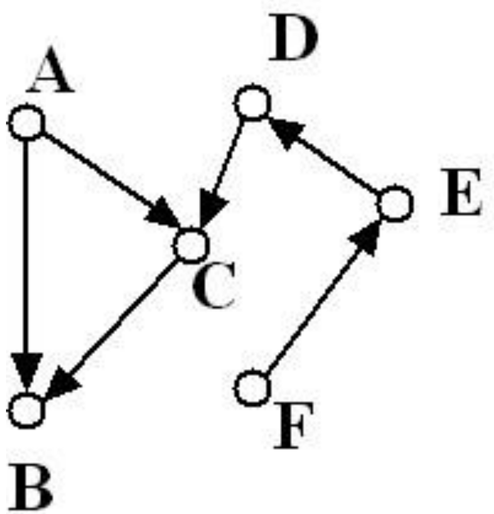
E.g. A, F are sources, B is a sink.

Average degree



$$\langle k \rangle \equiv \frac{1}{N}\sum_{i=1}^{N} k_i$$

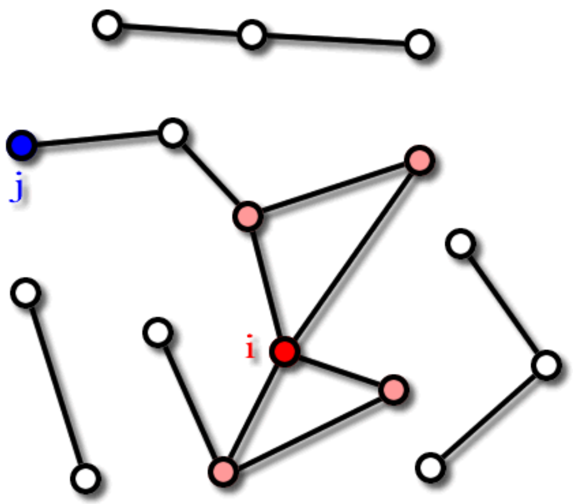
N – the number of nodes in the graph



$$\langle k^{in} \rangle \equiv \frac{1}{N}\sum_{i=1}^{N} k_i^{in}, \quad \langle k^{out} \rangle \equiv \frac{1}{N}\sum_{i=1}^{N} k_i^{out}, \quad \langle k^{in} \rangle = \langle k^{out} \rangle$$

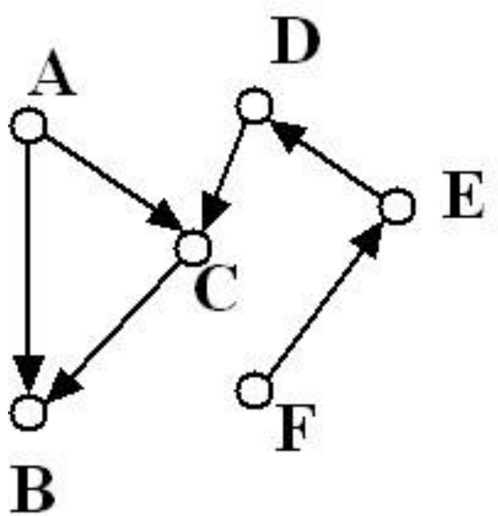
Q: What is the relation between the number of edges in a (non-directed) graph and the sum of node degrees? What about in a directed graph?

Statistics of node degrees



Average degree $\langle k \rangle \equiv \frac{1}{N}\sum_{i=1}^{N} k_i = \frac{2E}{N}$

$$\langle k^{in} \rangle = \langle k^{out} \rangle = \frac{E}{N}$$



The degree distribution $P(k)$ gives the fraction of nodes that have k edges.

Similarly $P(k^{in})$ / $P(k^{out})$ gives the fraction of nodes that have in-degree k^{in} / out-degree k^{out}.

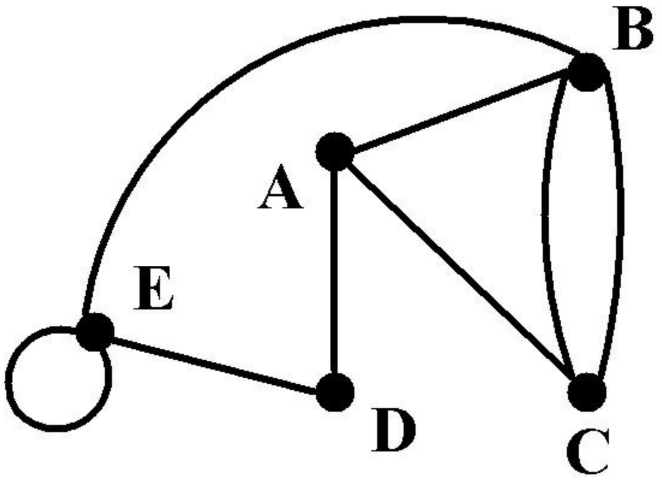
Ex. Calculate the degree distributions of the graphs in the left.

Exercise

Draw a graph or digraph with 4 nodes such that each node has degree one. Then repeat with degree two and three. Try to use a variety of edges: symmetrical, directed, multiple edges, loops.

Paths and circuits

Adjacent nodes (vertices) – there is an edge joining them.



Path: a sequence of nodes in which each node is adjacent to the next one.
Edges can be part of a path only once.

In the digraph framework the adjacency is only defined in the direction of the arrow.
A bidirectional edge can be used once in one direction and once in the opposite direction.

Circuit: a path that starts and ends at the same node.

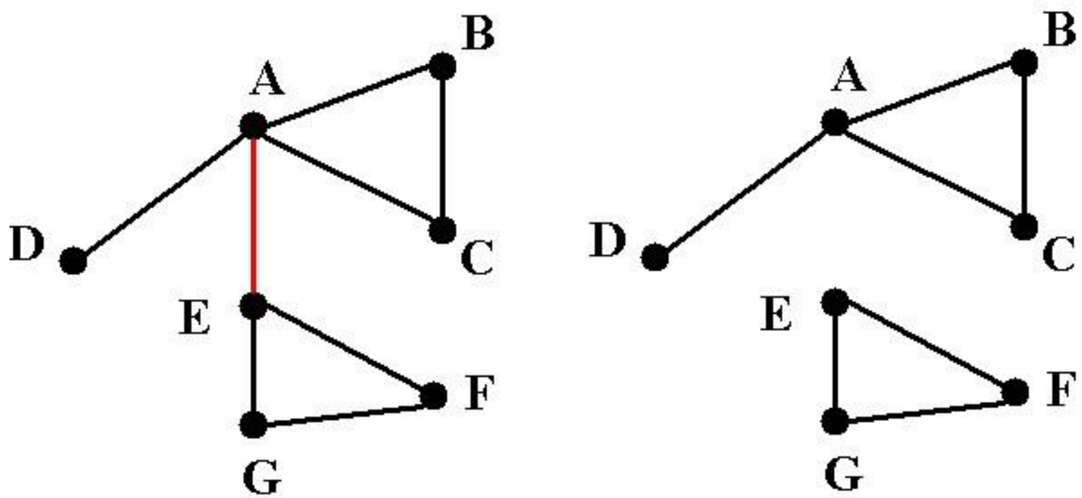
Cycle: a circuit that does not revisit any nodes.

Ex. Give examples of circuits and cycles in the above graph

Connectivity of undirected graphs

Connected (undirected) graph: any two nodes can be joined by a path.

A disconnected graph is made up by two or more connected components.



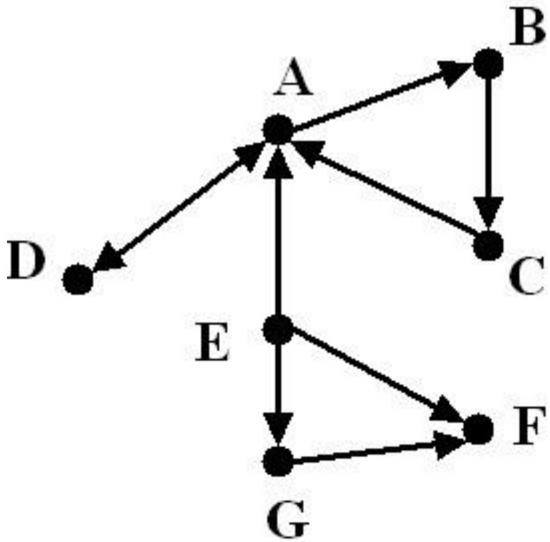
Bridge: if we erase it, the graph becomes disconnected.

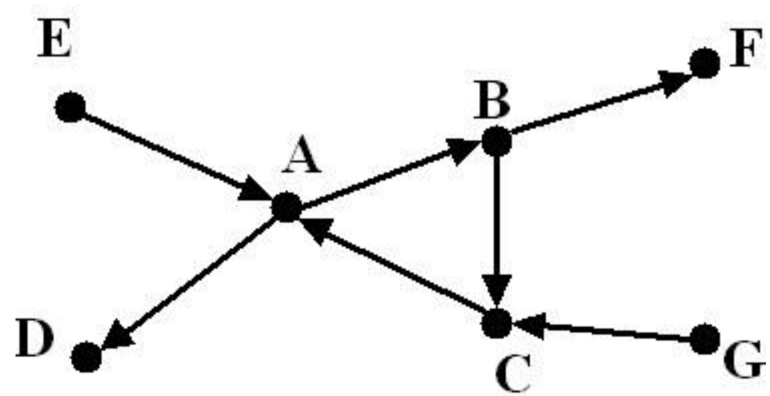
Q. Are there more bridges in the graph?
What is the smallest possible connected component?

Connectivity of directed graphs

Strongly connected directed graph: has a path from each node to every other node and vice versa (e.g. AB path and BA path).
Weakly connected directed graph: it is connected if we disregard the edge directions.

Strongly connected components can be identified, but not every node is part of a nontrivial strongly connected component.





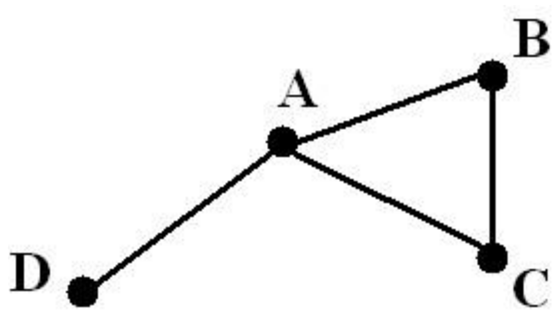
In-component: nodes that can reach the scc,
out-component: nodes that can be reached from the scc.

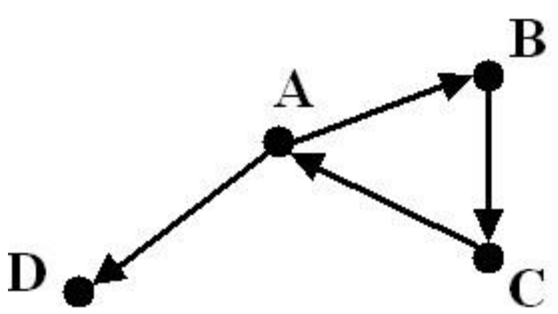
Exercises

1. You have N nodes and need to build a connected graph from them. Each time you add an edge you must pay \$1. What is the minimum amount of money needed to build the graph?

2. You are constructing a disconnected graph from N nodes. For each edge you add you receive \$1. You are not allowed to use directed edges, loops or multiple edges, and you must stop before the graph becomes connected. What is the most money you can make?

Distances between nodes





The distance between two nodes is defined as the number of edges along the shortest path connecting them.

If the two nodes are disconnected, the distance is infinity.

In digraphs each path needs to follow the direction of the arrows.

Thus in a digraph the distance from node A to B (on an AB path) is generally different from the distance from node B to A (on a BA path).

Ex. Calculate the distances among node pairs for the above graphs.

How to record distances

Tip: fill out the matrix

$$\begin{array}{ccccc} & A & B & C & D \\ A & 0 & l_{AB} & l_{AC} & l_{AD} \\ B & l_{BA} & 0 & l_{BC} & l_{BD} \\ C & l_{CA} & l_{CB} & 0 & l_{CD} \\ D & l_{DA} & l_{DB} & l_{DC} & 0 \end{array}$$

Q: How many non-zero entries will you need for an N- node graph?

A: N(N-1) in a digraph, N(N-1)/2 in a symmetrical graph. Let's use the notation

$$N_{pairs} = \binom{N}{2} = \frac{N(N-1)}{2}$$

Diameter and average distance

Graph diameter: the maximum distance between any pair of nodes in the graph. Note: not the longest path.

Average path length/distance for a connected graph (component) or a strongly connected (component of a) digraph.

$$\langle l \rangle \equiv \frac{1}{2N_{pairs}} \sum_{i,j \neq i} l_{ij}$$

, where l_{ij} is the distance from node i to node j, $N_{pairs} = \binom{N}{2} = \frac{N(N-1)}{2}$ and N is the number of nodes in the graph or component.

Since in a (symmetrical) graph $l_{ij} = l_{ji}$, we only need to count them once

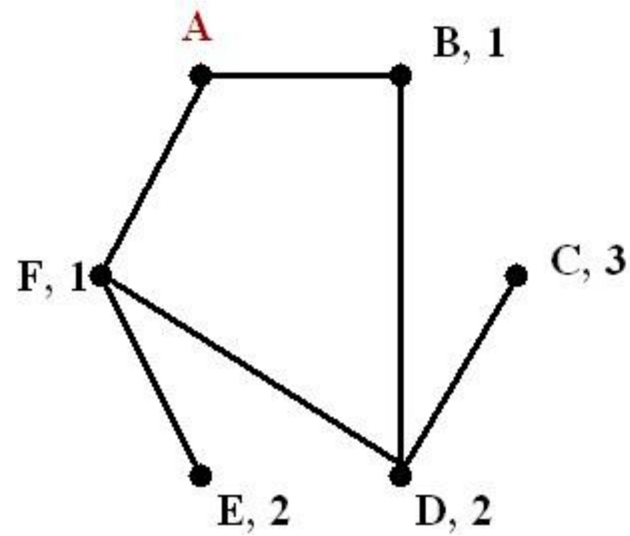
$$\langle l \rangle \equiv \frac{1}{N_{pairs}} \sum_{i,j>i} l_{ij}$$

Algorithm for finding distances- breadth first search

Distance between node u and node v:

1. Start at u.
2. Find the nodes adjacent to u. Mark them as at distance 1. Put them in a queue.
3. Take the first node, w, out of the queue. Find the unmarked nodes adjacent to it in the graph. Mark them with the label of w +1. Put them in the queue.
4. Repeat until you find v or there are no more nodes in the queue.
5. The distance between u and v is the label of v or, if v does not have a label, infinity.

Ex. Apply the algorithm to find the distance between A and C



Other applications of breadth first search

Find the connected components of a graph:

1. Start from a node u, label with 1
2. Find all nodes reachable from u, label with 1
3. Choose an unmarked node v, label with 2
4. Find all nodes reachable from v, label with 2
5. Repeat with increasing labels until no more unmarked nodes

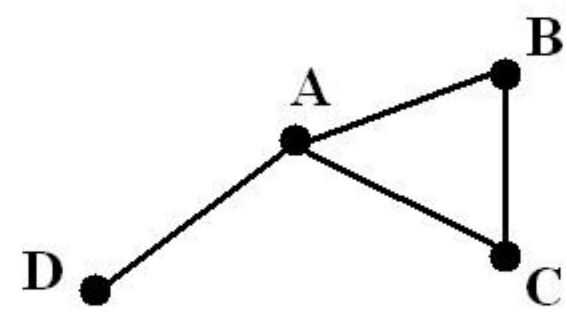
Calculate average distance of a connected graph:

1. Put the nodes in an ordered list
2. Use BFS to find distances between the first node and all other nodes, cumulate them
3. Use BFS to find distances between the second node and all other nodes except the first, cumulate them
4. Repeat as you go down the list
5. Divide cumulated distance by the number of node pairs

Graph efficiency

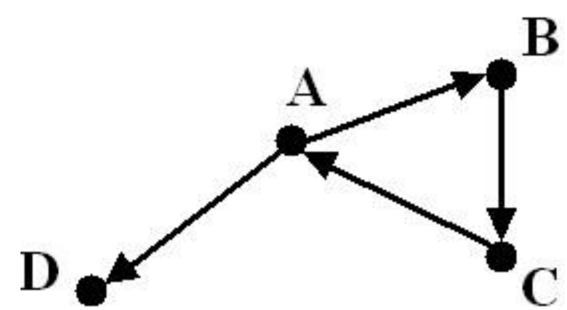
To avoid infinities in graphs that are not connected and digraphs that are not strongly connected, one can define a graph efficiency (= average inverse distance)

$$\eta \equiv \frac{1}{2N_{pairs}} \sum_{i,j \neq i} \frac{1}{l_{ij}}$$

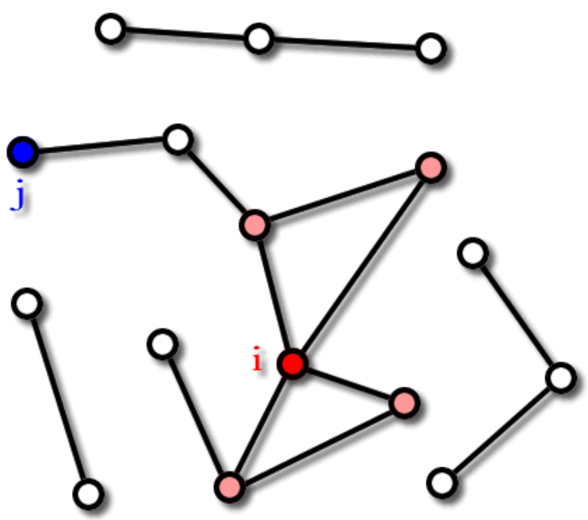


N_{pairs} is the number of node pairs

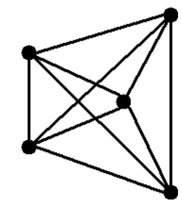
Ex.: Calculate the average distance and efficiency of the graphs on the right.



Local order and clustering



Clique: completely connected simple graph of N nodes and *N(N-1)/2* edges, *k=N-1* for each node



How close the neighborhood of a node is to a clique?

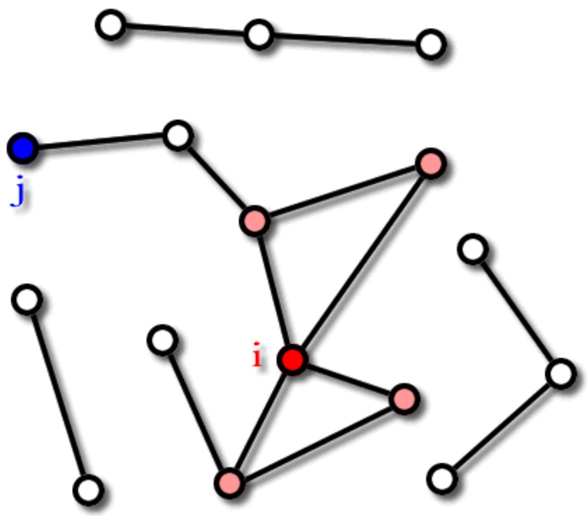
Edges among the nodes adjacent to *i*

Clustering coefficient

$$C_i \equiv \frac{n_i}{k_i(k_i-1)/2}, \quad k_i \neq 0,1$$ or

$$C_i \equiv \frac{nr.\ of\ triangles\ connected\ to\ \ i}{nr.\ of\ triples\ centered\ on\ i}$$

Clustering coefficient distributions



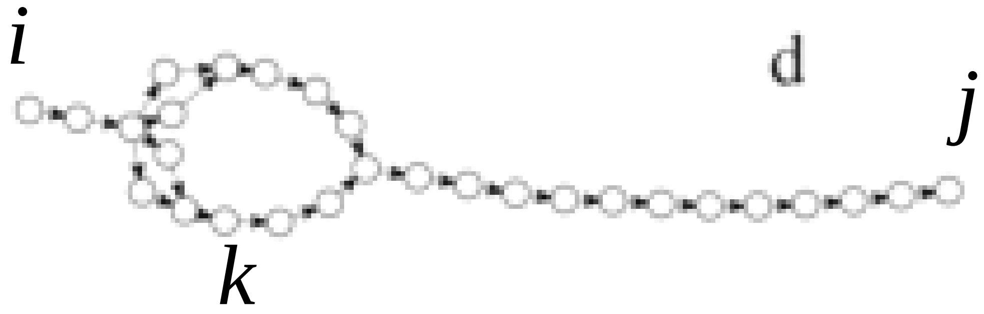
$$C_i \equiv \frac{n_i}{k_i(k_i-1)/2}, \quad k_i \neq 0,1$$

Clustering coefficient distribution: gives the fraction of nodes for each value (or range of values) of the clustering coefficient.

Clustering –degree function $C(k)$: for each degree>1 represented in the graph calculate the average clustering coefficient of the nodes with that degree.

Ex. Determine the clustering coefficient distribution and clustering-degree function of the above graph.

Betweenness centrality (load)



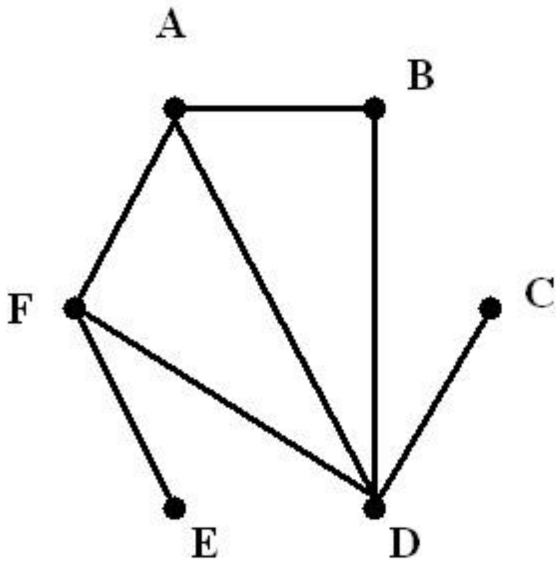
For all node pairs (*i*, *j*):

- Find all the shortest paths between nodes *i* and *j* - $C(i,j)$
- Determine how many of these pass through node k - $C_k(i,j)$

The betweenness centrality of node *k* is

$$g_k = \sum_{i \neq j} \frac{C_k(i,j)}{C(i,j)}$$

L. C. Freeman, Sociometry 40, 35 (1977)



$$g_k = \sum_{i \neq j} \frac{C_k(i,j)}{C(i,j)}$$

$C(i,j)$ –nr. of shortest paths btw. i,j
$C_k(i,j)$ – nr. of these paths that contain k

Ex1: Calculate the betweenness centrality of the nodes in this graph. Do not count being the starting or ending point of a path ($k \neq i$, $k \neq j$) .

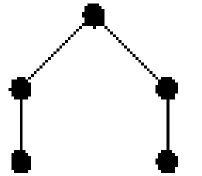
Tip: Construct a node pair (half)matrix and fill it with the nodes between each node pair.

Ex.2. Determine the betweenness centrality distribution for the graph.

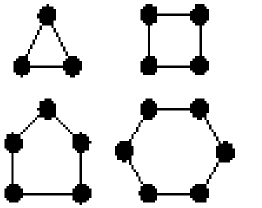
Common subgraphs

Subgraph: a subset of nodes of the original graph and of edges connecting them. Does not have to contain all the edges of a node included in the subgraph.

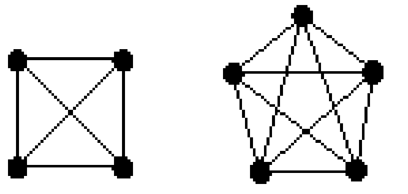
Trees: contain no circuits; N nodes and N-1 edges.



Cycles: circuits where nodes are not revisited;
N nodes and N edges



Cliques: completely connected subgraphs; N nodes
and N(N-1)/2 edges



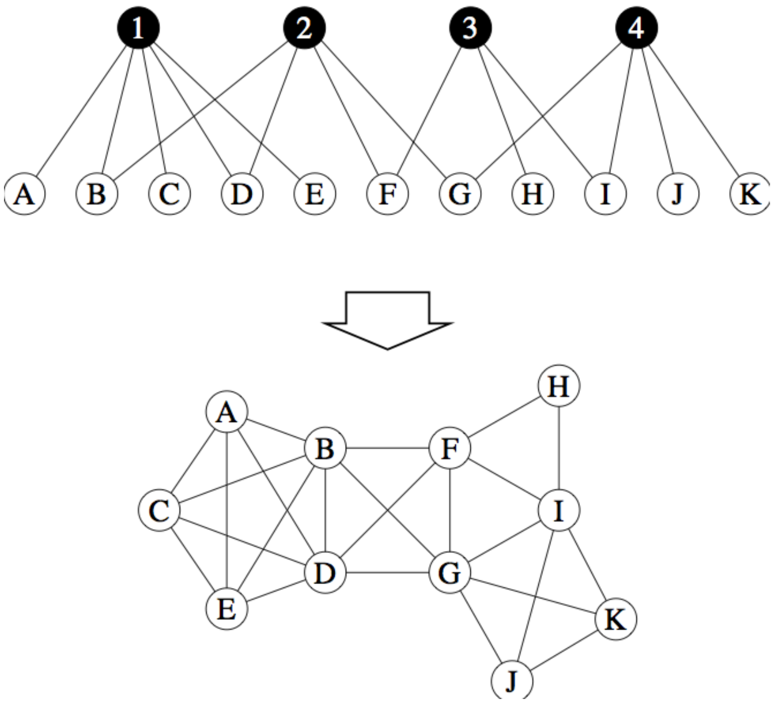
Note difference between connected and completely connected!

Bipartite graphs

Group structure (e.g. in social networks) can be incorporated into a bipartite graph.

A bipartite graph has two types of nodes:
group nodes (black, numbered)
member nodes (white, lettered)
Edges are possible only between different types of nodes: membership in group.

Two projections:
1. connect all members in a given group – each group becomes a completely connected subgraph
2. connect groups if they share members



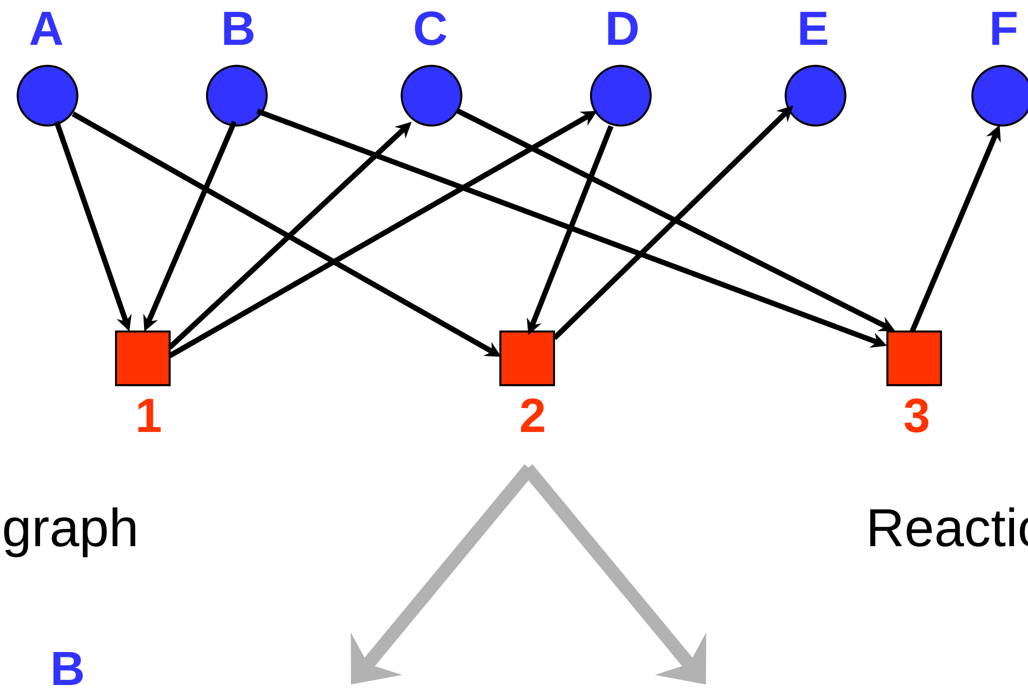
D. Watts, P. S. Dodds, M. E. J. Newman, Science 296 (2002)
M. E. J. Newman, S. Strogatz, D. Watts, Phys. Rev. E 64, 026118 (2001)

Q. What is your expectation for the average clustering coefficient of the member network (i.e. first projection) resulting from a bipartite graph?

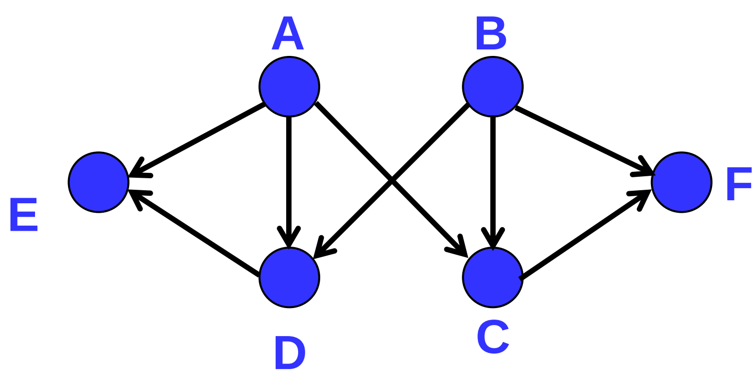
Ex. Represent these reactions by a bipartite graph.

$$A + B \rightarrow C + D \qquad (1)$$
$$A + D \rightarrow E \qquad (2)$$
$$B + C \rightarrow F \qquad (3)$$

Bi-partite Graph

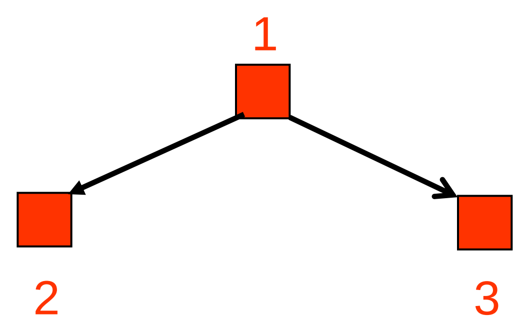


Molecule graph



Connect two molecules if there exists a 2-edge path in the bipartite graph between them

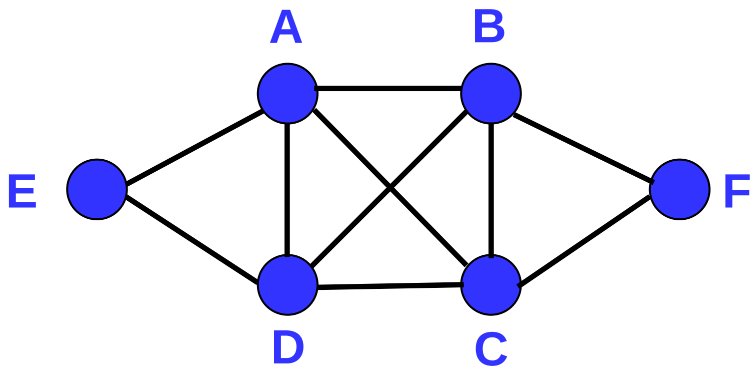
Reaction graph



Connect two reactions if there exists at least one 2-edge path in the bipartite graph between them

Ex. The early literature of metabolic networks used this type of representation:

Substrate Graph



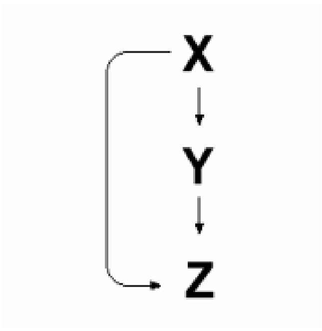
What information is preserved and what is lost?

A. Wagner & D. Fell, Proc. Roy. Soc. 268 (2001)

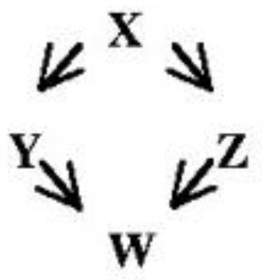
Special directed subgraphs

Bi-fan

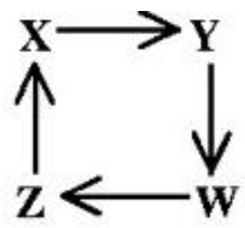
Feed-forward loop: two nonintersecting directed paths between a start and endpoint



Bi-parallel: two nonintersecting paths of identical length between a start and endpoint



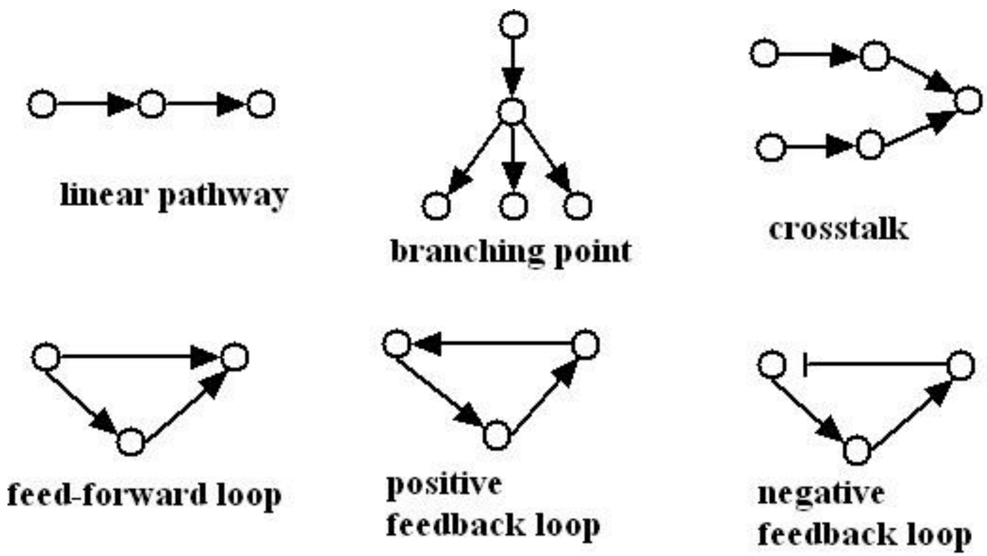
Feed-back loop: a directed cycle



S. S. Shen-Orr, R. Milo, S. Mangan and U. Alon, Nature Genetics (2002)

Network topology and dynamics

Network motifs can suggest regulatory relationships



Further, dynamic details are needed to describe how multiple inputs on a node are integrated - additive action (e.g. same product for two chemical reactions)

- synergy (e.g. transcriptional regulation)